

# **APPENDIX D. STEADY-STATE MODEL WORKBOOK AND USER GUIDE**

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### Attachment D-1. Steady-State Bioaccumulation Model Workbook

## Tables

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# 1 Overview

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This appendix presents the user with information for running the steady-state bioaccumulation model for the Lower Passaic River Study Area (LPRSA). The model, which is provided as Attachment D-1 of this Appendix, operates as a Microsoft Excel® workbook. Topics discussed in this appendix include the structure and layout of the model's workbook, important aspects of specific worksheets, information regarding how to operate the model, and common troubleshooting techniques that might be helpful to the user.

When first opening the workbook, there are some important items to note:

- ◆ Macros must be enabled for the workbook to function properly (Section 2.1).
- ◆ The workbook can be used to evaluate the impact on predicted tissue concentrations by modifying select input values in the bioaccumulation model and/or looking at results for different modeling areas (Section 2.2.1).
- ◆ Rows and columns should not be changed because of how they are referenced in the model code; changes in the workbook structure will cause errors and/or incorrect calculations (Section 2.4)
- ◆ The bioaccumulation model workbook consists of seven worksheets (one of which is hidden) and uses Microsoft Visual Basic for Applications® (VBA) code to calculate predicted tissue concentrations. Details regarding the content of the workbooks can be found in Section 3. Details regarding VBA and model code can be found in Section 2.3.

## 2 Workbook Operation

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This section discusses the operation of the bioaccumulation model workbook.

### 2.1 ENABLING MACROS

The LPRSA bioaccumulation model was developed using Microsoft Excel® 2007 and currently operates in Microsoft Excel® 2013. Macros, which must be enabled for the workbook to function properly, may be enabled using the following steps:

- ◆ On the File tab, choose the Options button.
- ◆ Under Excel Options, select Customize Ribbon.
- ◆ In the list of Main Tabs, check the Developer box and choose OK to exit the Excel Options dialog.
- ◆ On the Developer tab, select the Macro Security button.
- ◆ Under Macro Settings Options, check Enable All Macros and Trust Access to the VBA Project Object Model.

Once macros are enabled, the user will be able to run the model.

## 2.2 RUNNING THE MODEL

This workbook is dynamic, and any changes made to referenced input parameters will automatically update the model output.

### 2.2.1 Modifying the workbook

The bioaccumulation model workbook is designed to allow the user to modify select input values and/or look at model results for different modeling areas. The input values that can be modified by the user include the parameters that were calibrated, which are listed as follows:

- ◆ Dietary absorption efficiencies for invertebrates [eL, eP, eN]
- ◆ Octanol-water partitioning coefficient [ $K_{ow}$ ] for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) and tetraCB
- ◆ Species-specific metabolic biotransformation rate constants [ $K_M$ ] for 2,3,7,8-TCDD and tetraCB
- ◆ Carp particulate ventilation constants [CPV]

The user can evaluate the impact of changing these parameters by looking at the model performance metrics (i.e., the species-predictive accuracy factor [SPAF] and percent difference). To avoid potential issues associated with users modifying linked values (Section 3), cells for other parameters are locked so that these values cannot be changed.

### 2.2.2 Dropdown menus and buttons

Dropdown menus in the Output worksheet allow for the user to specify two options:

- ◆ Modeling area. Options included in this version of the model are site wide, river mile (RM) 4 to Dundee Dam, and RM 7 to Dundee Dam; modeling areas are discussed in Section 3.2.4 of the main report.
- ◆ Exposure assumption for small forage fish (i.e., whether small forage fish are exposed to river-wide concentrations or to mudflat-only concentrations).

The Record Model Output button runs a macro that records the date and time of the model run, key parameter settings, and model results from the Output worksheets onto the Output Record worksheet (Section 3.2.2). Runtime for this macro should be less than one minute (depending on computer processor speeds).

## 2.3 MODEL CODE

As discussed, model calculations are performed using VBA code, which uses the Excel® worksheets in the model workbook for input and output values. To view the model code, select the Developer tab within the ribbon and select the Visual Basic button (alternatively, Alt + F11 will also open the VBA code). The model code found within the Visual Basic Editor is responsible for the backend functions of the workbook; in order to maintain the functionality of the model, it should not be modified. The key portions of the model code include the following:

- ◆ Calculation of tissue concentrations
- ◆ Recording of output record (as described in Sections 2.2.2 and 3.2)
- ◆ Automatic re-calculation of model predictions

Appendix B provides a detailed description of the model code.

## 2.4 TROUBLESHOOTING

As discussed, it is important that no rows, columns, or cells are added or deleted in this workbook. Because of the way that cells are referenced in VBA code, the cell references do not update with changes to model structure; thus, the model will not operate correctly if the worksheet structure is modified.

An error reading #VALUE! might be seen in cells traditionally occupied by calculated and referenced values. To troubleshoot this error, select a new area from the dropdown menu in the Output worksheet, then return to the desired area. This operation enables the worksheet to return re-calculated and referenced values to the calculated and referenced cells.

## 3 Workbook Structure

The steady-state bioaccumulation model is contained in an Excel® workbook that includes seven worksheets. This workbook allows for the automated calculation of bioaccumulation in biota tissue based on a variety of input parameters. The workbook should be treated as static due to the stationary nature of the VBA code that backs the workbook. The insertion, deletion, or movement of cells, columns, or rows may prevent the model from performing correctly.

The following subsections describe the seven model worksheets, which are labeled Output, Output Record, Diet, BC (blue crab), Chemical Input, Empirical Tissue, and Index.

### 3.1 WORKSHEET 1: OUTPUT

There are two main parts to this worksheet: model inputs and model outputs.

#### 3.1.1 Model inputs

The Output worksheet contains four of the types of model input parameters needed to run the bioaccumulation model: chemical-specific parameters, general physical parameters, general biological parameters, and species-specific parameters. The inputs in this worksheet may be entered as static values (i.e., the parameter value is entered directly into this worksheet) or as linked values (i.e., the cell references a value in another worksheet). All input values are shaded orange. Table 3-1 summarizes the parameters included in the “Output” worksheet.

**Table 3-1. Summary of parameters on the “Output” worksheet**

Parameters Name	FWM Code	Type	Calibrated?
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<b>Chemical-specific parameters</b>			
Octanol-water partition coefficient	K <sub>ow</sub>	static	yes
Concentration in sediment solids	CST	linked value <sup>a</sup>	no
Concentration in detrital particulates	CPART	linked value <sup>a</sup>	no
Bioavailable concentration in water	CWB	linked value <sup>a</sup>	no
Concentration in sediment porewater	CSD	linked value <sup>a</sup>	no
Concentration in near-bottom particulates	CFL	linked value <sup>a</sup>	no
<b>General physical parameters</b>			
OC content of sediment	OCSS	linked value <sup>a</sup>	no
OC content of detrital particulate	OCPart	linked value <sup>a</sup>	no
OC content of near-bottom particulates	OCPart_Det	linked value <sup>a</sup>	no
Mean water temperature	TW	linked value <sup>a</sup>	no
<b>General biological parameters</b>			
Uptake constant A for organism	UA	static	no
Uptake constant B for organism	UB	static	no
Dietary transfer efficiency constant A	EDA	static	no
Dietary transfer efficiency constant B	EDB	static	no
NLOM-octanol proportionality constant	BETA	static	no
NLOC-octanol proportionality constant	GAMMA	static	no
<b>Species-specific parameters</b>			
Growth rate constant	KG	static	no
Weight	WB	static	no
Lipid fraction of organism	VLB	static	no
Water content fraction of organism	VWB	static	no
NLOC fraction of organism	VPB	static	no
NLOM fraction of organism	VNB	static	no
Dietary absorption efficiency of lipid	eL	static	invertebrates only
Dietary absorption efficiency of NLOC	eP	static	invertebrates only
Dietary absorption efficiency of NLOM	eN	static	invertebrates only
Dietary absorption efficiency of water	eW	static	no
Fraction of pore water ventilated	FPW	static	no
Particulate ventilation constant	CPV	static	yes
Metabolic biotransformation rate constant (2,3,7,8-TCDD)	K <sub>M</sub>	static	yes
Metabolic biotransformation rate constant (tetraCB)	K <sub>M</sub>	static	yes

<sup>a</sup> Values are linked to the chemical inputs tab and depend on the selected dropdown options. These values originate from the CFT model developed by Anchor QEA.

CFT – contaminant fate and transport

NLOC – non-lipid organic carbon

NLOM – non-lipid organic matter

OC – organic carbon  
TCDD – tetrachlorodibenzo-*p*-dioxin

### 3.1.2 Model outputs

Model-predicted tissue concentrations are also provided in the Output worksheet. These values are located in cells E70:P70 (2,3,7,8-TCDD), E98:P98 (tetraCB), and E169:P169 (total polychlorinated biphenyls [PCBs]). Tissue concentrations for total PCBs are calculated from predicted tetraCB concentrations using three different regressions (discussed in Section 3.4.3 of the main report and in Appendix J). In the rows immediately below the predicted tissue concentrations for each chemical, the average empirical tissue concentrations are shown; these values are linked to the Empirical Tissue worksheet. The model performance metrics (SPAF and percent difference) are both calculated values and are found in the two rows following the empirical tissue concentrations.

Rows 74:94 and 102:157 are currently hidden in this worksheet. These rows are placeholders for output for other PCB homologs in the event that model predictions are added later for these chemicals.

## 3.2 WORKSHEET 2: OUTPUT RECORD

As discussed in Section 2.2.2, the Record Model Output function of the workbook records relevant parameter settings, records model output, and generates summary figures using these data. This record of the model run is recorded in the Output Record worksheet.

### 3.2.1 Parameter settings

The parameters for which values are recorded include the  $K_{ow}$ , metabolic biotransformation rate constants, and dietary absorption efficiency for invertebrates. These parameters were modified during model calibration.

### 3.2.2 Model outputs

Model outputs are recorded in the same format as in the Output worksheet. Modeled tissue concentrations can be found in cells E15:P15 (2,3,7,8-TCDD), E22:P22 (tetraCB), and E26:P26 (total PCBs). Tissue concentrations for total PCBs are calculated from model-predicted tetraCB concentrations using site-specific regressions (Appendix J). The rows below the predicted tissue concentrations show the empirical tissue concentrations, SPAFs, and percent differences.

In addition to these results, this tab presents three sets of tables:

- ◆ **Target concentrations tables** – These tables (one for 2,3,7,8-TCDD and one for tetraCB) present model-predicted concentrations, and a comparison with the 25<sup>th</sup> and 75<sup>th</sup> percentiles of the empirical data.
- ◆ **Inputs table** – This table summarizes the values for the key parameters values for the current model run, and compares them to the distribution values.
- ◆ **SPAF table** – This table presents the SPAFs for the target species based on

the current model run.

### 3.2.3 Plots

Using the tables discussed, plots were made to illustrate model performance and parameter settings of the current calibration. These plots include the following:

- ◆ **Percent Difference 2,3,7,8-TCDD and Percent Difference TetraCB** – These first two plots compare the percent difference of the predicted concentrations to the average empirical concentration to evaluate whether the model is under- or over-predicting the tissue concentration.
- ◆ **Parameter Settings** – This plot compares the current parameter values for the invertebrate absorption efficiencies and species-specific metabolic biotransformation rate constants to the distribution ranges.
- ◆ **Predicted vs. Empirical (for both 2,3,7,8-TCDD and tetraCB)** – These plots compare the predicted values to empirical data ranges for 2,3,7,8-TCDD and tetraCB.
- ◆ **SPAFs** – This plot compares the SPAFs for each species and chemical and shows the over- and under-prediction of the modeled tissue concentrations for the target species.

### 3.3 WORKSHEET 3: DIET

The Diet worksheet contains the diet fraction parameter values for species-specific predator and prey relationships among 12 of the 13 modeled compartments.

There are two portions of this worksheet. The upper portion (rows 2:14) contains calculated values, which ensure that the diet fractions are normalized to a total of 100% for each modeled species. The lower portion (rows 16:25) contains the cells where diet fractions are entered. Within this table, cells shaded in purple or blue contain calculations that reference values in rows 35:43 (for invertebrate prey items) and rows 46:51 (for fish prey items). For reference, rows 27:28 present the model-predicted concentrations for the various prey items for both 2,3,7,8-TCDD and tetraCB. The cells in these rows are shaded in pink to reflect the magnitude of the concentrations.

### 3.4 WORKSHEET 4: BC

The BC worksheet contains input and output data for blue crab; these data are separate from data for the rest of the modeled species because blue crab was incorporated into the bioaccumulation model at a later date. The organization of this worksheet is similar to that of the Output worksheet (Section 3.1), except that the BC worksheet also contains the prey portions for blue crab (presented in a format similar to that of the Diet worksheet). In addition, this worksheet also presents a figure comparing the predicted blue crab tissue concentrations with the empirical data for the three modeled chemicals.

### **3.5 WORKSHEET 5: CHEMICAL INPUTS**

The Chemical Inputs worksheet contains data from the contaminant fate and transport (CFT) model that is used by the steady-state bioaccumulation model to predict tissue concentrations (see Appendix C for a description of how CFT model data are used in the bioaccumulation model). Chemical input data from the CFT model are formatted in a specific way relative to river areas, parameters, and river sections. The format of this data worksheet should not be varied because it is referenced by other worksheets in the workbook.

### **3.6 WORKSHEET 6: EMPIRICAL TISSUE**

The Empirical Tissue worksheet contains the empirical tissue concentration data that were used to calibrate and evaluate model performance (Windward 2010, [in prep]). Values in this worksheet are referenced by other worksheets and are used to calculate performance metrics of SPAFs and percent difference. The format of this worksheet and its values should not be modified.

### **3.7 WORKSHEET 7: INDEX**

The Index worksheet is an additional tab that can be unhidden in the bioaccumulation model. This worksheet acts as an index, allowing various functions to reference values used for a calculation or function. The format of this worksheet and its values should not be modified.

## 4 References

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- Windward. 2010. Fish and decapod field report for the late summer/early fall 2009 field effort. Final. Prepared for the Cooperating Parties Group, Newark, NJ. September 14, 2010. Lower Passaic River Restoration Project. Windward Environmental LLC, Seattle, WA.
- Windward. [in prep]. 2010 small forage fish tissue chemistry data for the Lower Passaic River Study Area. Draft. Prepared for Cooperating Parties Group, Newark, NJ. Submitted to USEPA July 18, 2012. Lower Passaic River Restoration Project. Lower Passaic River Study Area RI/FS. Windward Environmental LLC, Seattle, WA.